

WEST Search History

DATE: Monday, May 10, 2004

<u>Hide?</u>	<u>Set Name</u>	<u>Query</u>	<u>Hit Count</u>
<i>DB=PGPB,USPT; PLUR=YES; OP=ADJ</i>			
<input type="checkbox"/>	L12	l11 and catechol	0
<input type="checkbox"/>	L11	l6 and l10	6
<input type="checkbox"/>	L10	polymerization inhibitor	8729
<input type="checkbox"/>	L9	l6 and l8	1
<input type="checkbox"/>	L8	cyclohexanecarbonyl chloride	463
<input type="checkbox"/>	L7	cyclohexanevarbonyl chloride	0
<input type="checkbox"/>	L6	l5 and (chlorinat\$ or halogenat\$)	30
<input type="checkbox"/>	L5	l4 and hydrogenat\$	37
<input type="checkbox"/>	L4	l3 and carboxylic acid	93
<input type="checkbox"/>	L3	l2 and acrylic acid	139
<input type="checkbox"/>	L2	l1 and \$butadiene	176
<input type="checkbox"/>	L1	cyclohexyl phenyl ketone	539

END OF SEARCH HISTORY

WEST Search History

DATE: Monday, May 10, 2004

Hide? **Set Name** **Query** **Hit Count**

DB=PGPB,USPT; PLUR=YES; OP=ADJ

☐ L3 12 and acrylic acid 0

☐ L2 11 and butadiene 11

☐ L1 cycloalkyl aryl ketone\$ 17

END OF SEARCH HISTORY

=> d his

(FILE 'HOME' ENTERED AT 22:52:08 ON 10 MAY 2004)

FILE 'CASREACT' ENTERED AT 22:52:27 ON 10 MAY 2004

L1 STRUCTURE UPLOADED

L2 0 S L1

L3 25 S L1 FULL

FILE 'CAPLUS' ENTERED AT 22:53:40 ON 10 MAY 2004

L4 5256 S ?PHENYL KETONE?

L5 1033 S L4 AND CYCLOHEX?

L6 76 S L5 AND ?DIENE

L7 5 S L6 AND ACRYLIC ACID

L8 204 S L4 AND ?DIENE

L9 13 S L8 AND ACRYLIC ACID

L10 20 S L4 AND DIELS-ALDER?

L11 2 S L10 AND ?CARBOXYLIC ACID

L12 372 S L4 AND ?CARBOXYLIC ACID

L13 16 S L12 AND (HALOGENAT? OR CHLORINAT?)

L14 3 S L13 AND HYDROGENAT?

L15 170 S L12 AND ?CHLORIDE

L16 4994 S POLYMERIZATION INHIBITOR?

L17 385 S L16 AND ?CATECHOL

L18 0 S L12 AND L17

L19 2 S L8 AND ?CATECHOL

L20 1 S L13 AND ?CATECHOL

L21 2 S L6 AND ?CATECHOL

L14 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:307622 CAPLUS

DOCUMENT NUMBER: 140:303405

TITLE: Preparation of cyclohexyl **phenyl ketone** from 1,3-butadiene and acrylic acid without purification of intermediates

INVENTOR(S): Ju, Yeong-je; Kim, Jin-eok; Won, Jeong-im; Kan, Tae-yi

PATENT ASSIGNEE(S): Korea Kumho Petrochemical Co., Ltd., S. Korea

SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

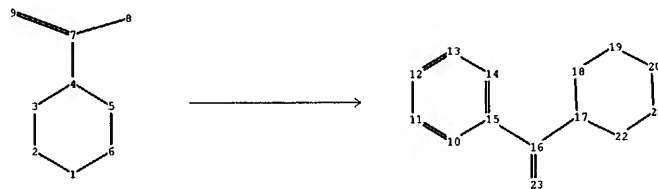
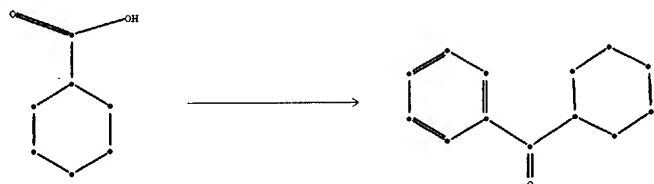
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2004115499	A2	20040415	JP 2003-201414	20030724
US 2004073068	A1	20040415	US 2003-628800	20030728

PRIORITY APPLN. INFO.: KR 2002-58627 A 20020927

AB Cyclohexyl Ph ketone, useful as an intermediate for photoinitiator 1-hydroxycyclohexyl Ph ketone (no data), is prepared by [2+4] Diels-Alder reaction of 1,3-butadiene with acrylic acid in the presence or absence of solvents, **hydrogenation** of 3-cyclohexene-1-**carboxylic acid**, without purification, **chlorination** of the resulting **cyclohexanecarboxylic acid** solution, and without separation of intermediate chloride and byproducts, Friedel-Crafts reaction of the chloride in the same reactor. Acrylic acid was reacted with 1,3-butadiene in the presence of 4-tert-butylcatechol in benzene at 120° for 2 h, **hydrogenated** using Pd/C under 120 psi H at 100°, and **chlorinated** with SOCl₂ in benzene under reflux for 1 h to give cyclohexanecarbonyl chloride, which was treated with AlCl₃ under reflux for 1 h to give cyclohexyl Ph ketone with ≥99% selectivity at 99% conversion.



```

chain nodes :
  7  8  9 16 23
ring nodes :
  1  2  3  4  5  6 10 11 12 13 14 15 17 18 19 20 21 22
chain bonds :
  4-7  7-8  7-9 15-16 16-17 16-23
ring bonds :
  1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15
  17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
  16-23
exact bonds :
  1-2 1-6 2-3 3-4 4-5 4-7 5-6 15-16 16-17 17-18 17-22 18-19
  19-20 20-21 21-22
normalized bonds :
  7-8 7-9 10-11 10-15 11-12 12-13 13-14 14-15
isolated ring systems :
  containing 1 : 10 : 17 :

Match level :
  1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
 10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:Atom
 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:CLASS
fragments assigned product role:
  containing 10
fragments assigned reactant/reagent role:
  containing 1
  
```

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 22:52:49 FILE 'CASREACT'

SCREENING COMPLETE - 31 REACTIONS TO VERIFY FROM 5 DOCUMENTS

100.0% DONE 31 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED VERIFICATIONS: 286 TO 954

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 full

FULL SEARCH INITIATED 22:52:54 FILE 'CASREACT'

SCREENING COMPLETE - 600 REACTIONS TO VERIFY FROM 105 DOCUMENTS

100.0% DONE 600 VERIFIED 60 HIT RXNS 25 DOCS

SEARCH TIME: 00.00.01

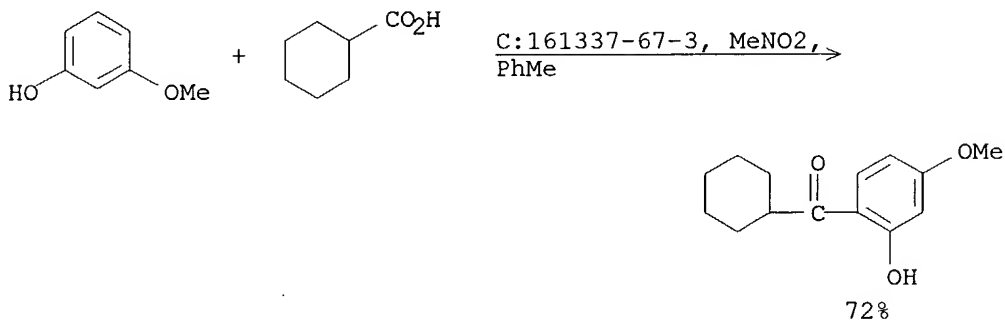
L3 25 SEA SSS FUL L1 (60 REACTIONS)

=> d scan

L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI Catalytic direct C-acylation of phenol and naphthol derivatives using
carboxylic acids as acylating reagents

RX(4) OF 4



NOTE: regioselective

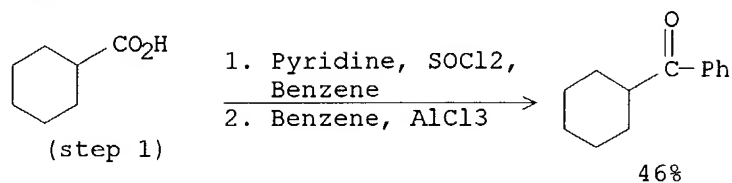
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI Synthesis and structure-activity relationships of potential

anticonvulsants based on 2-piperidinecarboxylic acid and related pharmacophores

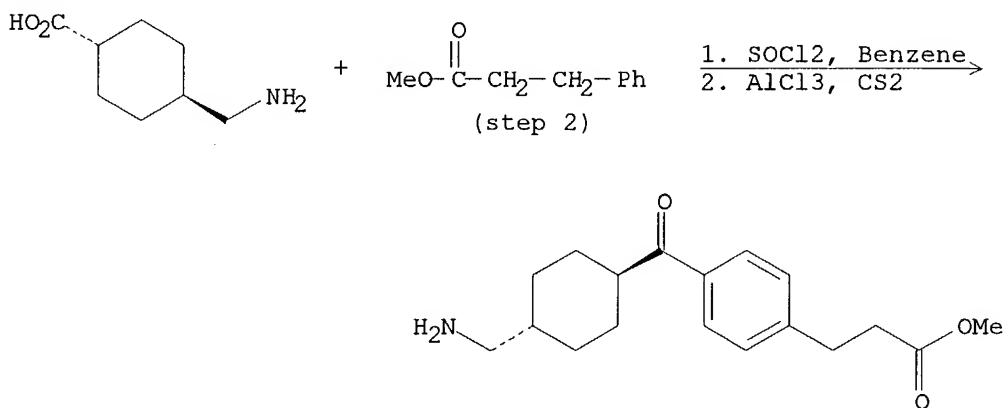
RX(2) OF 193



L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI A facile synthesis of aminocarboxylic acid derivatives, new anti-ulcer agents

RX(8) OF 13 - 2 STEPS

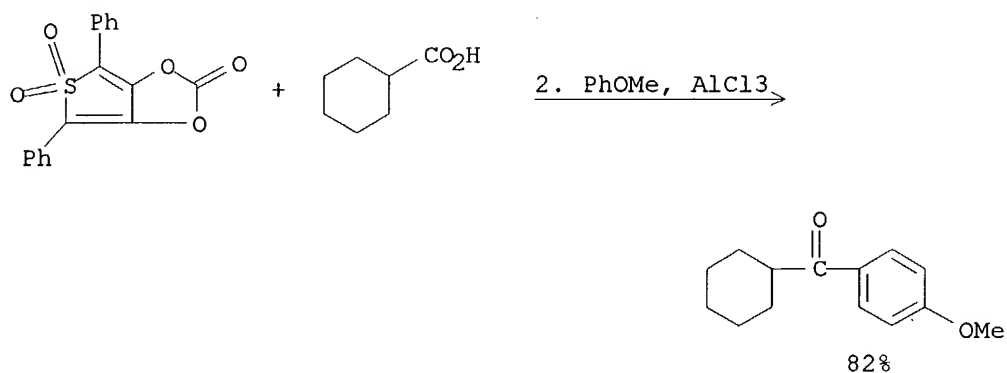


HCl

L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI 4-Acyloxy-2,5-diphenyl-3-oxo-2,3-dihydrothiophene 1,1-dioxides as acylating agents in the Friedel-Crafts reaction

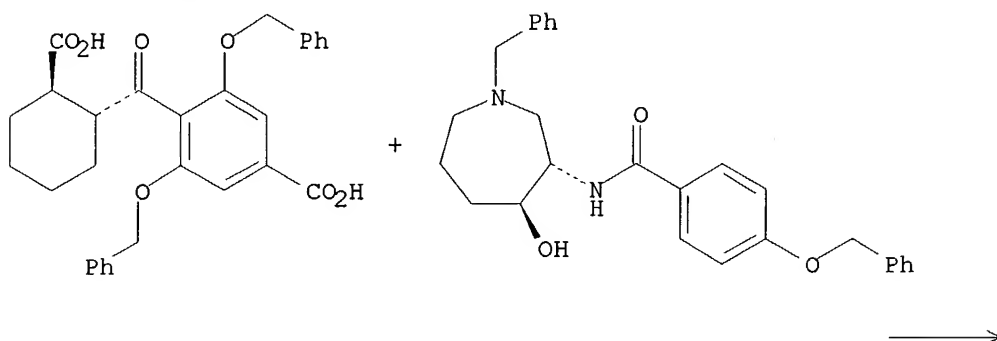
RX(35) OF 47 - 2 STEPS



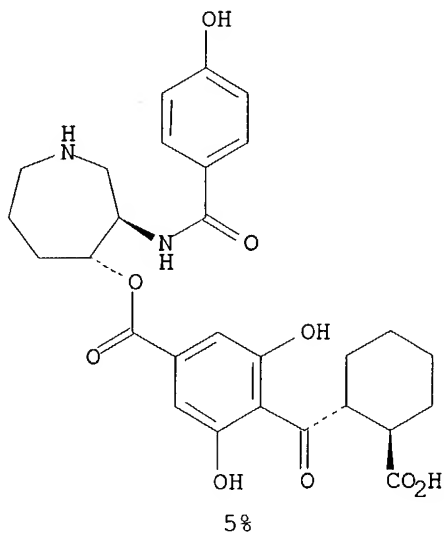
L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI Synthesis and Protein Kinase Inhibitory Activity of Balanol Analogues with Modified Benzophenone Subunits

RX(77) OF 305



RX(77) OF 305

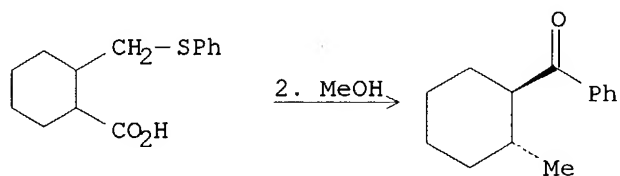


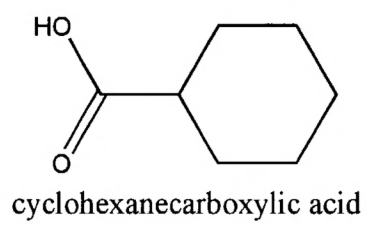
NOTE: general procedure available

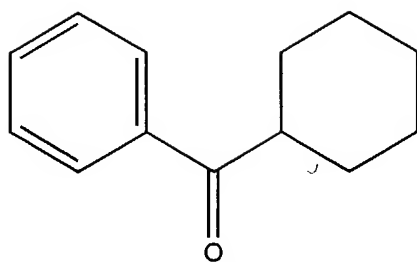
L3 25 ANSWERS CASREACT COPYRIGHT 2004 ACS on STN

TI Syntheses of 6,6a,7,8,9,10,10a,11-octahydro-11-oxodibenz[b,e]oxepins and 6,6a,7,8,9,10,10a,11-octahydro-11-oxodibenzo[b,e]thiepins

RX(11) OF 14 - 2 STEPS







cyclohexyl phenyl ketone